1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{21}\text{H}_{21}\text{F}_{3}\text{N}_{6}\text{O}_{2} \cdot \frac{1}{2}\text{H}_{2}\text{O} \)

Batch Molecular Weight: 455.44

Physical Appearance: White solid

Solubility: DMSO to 5 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: \( R_f = 0.5 \) (Dichloromethane:Methanol [9:1])

HPLC: Shows >99.5% purity

\(^1\text{H NMR:} \) Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

<table>
<thead>
<tr>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>55.38</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>4.87</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>18.45</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: GS 6201
Catalog No.: 4727
Batch No.: 4

CAS Number: 752222-83-6
IUPAC Name: 3-Ethyl-3,9-dihydro-1-propyl-8-[1-[[3-(trifluoromethyl)phenyl]methyl]-1H-pyrazol-4-yl]-1H-purine-2,6-dione

Description:
Selective antagonist of adenosine A$_{2B}$ receptors (K$_i$ values are 22, 1070, 1940 and 3280 nM for human A$_{2B}$, A$_3$, A$_1$ and A$_{2A}$ receptors respectively). Attenuates allergen-, NECA- and AMP-induced airway reactivity in an allergic mouse model of asthma. Also shown to attenuate the inflammatory response during acute myocardial infarction in mice; reduces caspase-1 activity in the heart.

Physical and Chemical Properties:
Batch Molecular Formula: C$_{21}$H$_{21}$F$_3$N$_6$O$_2$·½H$_2$O
Batch Molecular Weight: 455.44
Physical Appearance: White solid
Minimum Purity: >99%

Storage: Store at -20°C

Solubility & Usage Info:
DMSO to 5 mM

Stability and Solubility Advice:
Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:
SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.
SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

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